# LA-UR- 99-5359

Approved for public release; distribution is unlimited.

Author(s):

David S. DeCroix, William S. Smith, Gerald E. Streit, Michael J. Brown

Submitted to:

11th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association, Long Beach, California, 9-14 January 2000.

# Los Alamos

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# LARGE-EDDY AND GAUSSIAN SIMULATIONS OF DOWNWIND DISPERSION FROM LARGE BUILDING HVAC EXHAUST

David S. DeCroix\*, William S. Smith, Gerald E. Streit, and Michael J. Brown Los Alamos National Laboratory, Los Alamos, New Mexico

## 1.0 Introduction

In the event of smoke or a pollutant released at a large indoor event, the pollutant would diffuse throughout the interior of the building and would likely be exhausted to the atmosphere through the heating, ventilation and air conditioning (HVAC) ducts, thus exposing the population in the vicinity of the building. As this is a conceivable urban event, we have simulated such a scenario for a large building, typical of sports or convention centers. We have not modeled dispersion in the interior of the building, but rather have specified a continuous release of a massless tracer for a finite duration at the location of the HVAC vents.

These simulations are of a single building with flat terrain in neutral stratification, using the HIGRAD large-eddy simulation (LES) code. This code is in the process of being validated against wind tunnel experiments at the EPA FMF (Environmental Protection Agency Fluid Modeling Facility). Preliminary test and validation results are being presented at this conference, (Brown et.al. 2000, Smith et.al. 2000). The HIGRAD model was used to determine the near-source dispersion, and these results were then used to initialize the source description for the intermediate range Gaussian puff model, INPUFF, and a Gaussian plume model.

## 2.0 Model Description and Setup

The accurate simulation of the transport of a tracer released into an urban area requires sufficiently high model resolution (1-10 m grid cells) to resolve buildings and urban street canyons. At LANL, an effort has been underway to develop a model capable of simulating flow at the high spatial resolution required within the urban environment. HI-GRAD uses state-of-the-art numerical techniques to accurately simulate the regions of strong shear found near edges of buildings (Smolarkiewicz and Grabowski, 1990; Smolarkiewicz

\*Corresponding Author: David S. DeCroix, Los Alamos National Laboratory, Group TSA-4, Mail Stop F604, Los Alamos, NM, 87545.

Email: ddecroix@lanl.gov

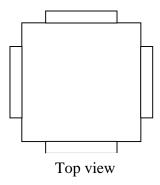
and Margolin, 1993; Smolarkiewicz and Margolin, 1994). HIGRAD is a large-eddy simulation code, second-order accurate in space and time, uses a terrain following coordinate system, has an optional solar radiation physics package (to include building shading effects), and one may use either a Smagorinsky (Smagorinsky, 1962) or turbulent kinetic energy (TKE) based (Sorbjan, 1996) subgrid closure scheme. In addition to the equations of motion and state, a separate prognostic equation is solved for each tracer source, corresponding to 16 additional equations for this simulation. The results presented in this paper use the Smagorinsky closure scheme and have no building shading effects.

The modeled building is approximately cubical with a "wing" on each side. There are four HVAC exhaust vents per side, two on the front of each wing, and one on either side of the wing, for a total of 16 modeled exhaust vents. The main section of the building is approximately 100*m* on each side, and 50*m* high, and each wing is approximately 45*m* high, 60*m* wide, and 10*m* deep (L=120m, H=50*m*). Figure 1 shows the top and side views of the building shape being modeled; the HVAC exhaust vents are shown as the shaded regions.

The computational domain used in these simulations was 14L x 7L x 5H in length, width, and height, (X, Y, and Z) respectively, or 1680 x 840 x 250m. The building was placed such that the domain extended 3H upstream and 10H downstream of the building. For the initial simulations, the grid resolution was uniform at 10m in the lateral directions and 5m in the vertical. The inflow conditions simulated were those of a typical winter day, neutral stratification, low turbulence intensity, and a mean flow velocity profile with a power law form:

 $U = 3.5 * (Z/250)^{0.16}$ 

This produces a wind speed of approximately 2.7 *m*/s at the top of the building.



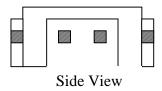


Figure 1. Top and side view schematic of the building. The HVAC exhaust is shown as the shaded area.

#### 3.0 Discussion of HIGRAD Simulation Results

The flow field was allowed to develop for 30 minutes, then the tracer was released for 10 minutes, and the integration was continued for an additional 20 minutes, for a total simulation time of 60 minutes. There were sixteen massless tracer release points corresponding to the actual HVAC exhaust locations. The tracer was continuously emitted for 10 minutes (starting at T=30 minutes) at a rate of 1 unit mass per unit volume per time step.

Figures 2 (a-f) show the instantaneous concentration contours at the height of the vents, Z=35m. Figure 2a is at T=35 minutes, or 5 minutes after the start of the release, Figure 2b is at T=40 minutes, precisely when the tracer is turned off, and figures 2c through 2f are at T= 45, 50, 55, and 60 minutes respectively. The dispersion shown is non-Gaussian with a substantial amount of the tracer trapped in the building recirculation zone. The concentration contours that seem to not to be connected to the building wake region are due to the vents located on the upstream side. The tracer is advected around the corner of the building, most of which is advected downstream, but some is advected and diffused laterally due the blockage effect. There is a vortex on each side of the building that is ingesting fresh air from above, and at this height the contours appear separate. At lower elevations the concentration contours are more continuous.

Also, there is very little evidence of a roof top recirculation bubble. This is likely due to the presence of the "wings", but may be due to inadequate grid resolution. Another study with double this simulation's resolution is underway and these results will be presented at the conference. We wish to answer whether the roof top bubble is missing due to resolution constraints or because of the geometry being modeled. This will also allow us to assess the effects subgrid closure scheme on the simulation results.

## 4.0 Results of the Gaussian Dispersion Models

The Gaussian puff model, INPUFF (Petersen and Lavdas 1986), was applied to the simulation of the downwind dispersion of a tracer released from the air exhaust vents of the same large building. The simple application assumed one roof-level source. The more complex application drew from HIGRAD CFD results to develop the descriptions of multiple sources, each with the appropriate initial  $\sigma_v$  and  $\sigma_z$ , the lateral and vertical plume spread parameters, respectively, to better simulate the plume behavior close to the building. Though only one case has been examined so far, the intent is to generalize some urban effects for use in a relatively simple, quick-running model so that public safety personnel can make rapid assessment of the hazard level and hazard zones. Figure 3 shows qualitatively the effect of a building on plume dispersion. A plume from an elevated source with no building effects will travel some distance downwind before it impacts the ground. With the same elevated source accompanied by building effects, the effects of the building cavity and recirculation will bring plume material to ground level directly behind the building and increased turbulence will enhance plume dispersion.

# 4.1 INPUFF Model Description

INPUFF (Integrated PUFF) may be used to simulate dispersion from nearly instantaneous or continuous sources. A vertically uniform wind direction is assumed, but the wind field may be spatially or temporally variable. The source may be a point, or multiple points to simulate a line source, or spatially distinct point sources. There are no chemical reactions, but gravitational settling and

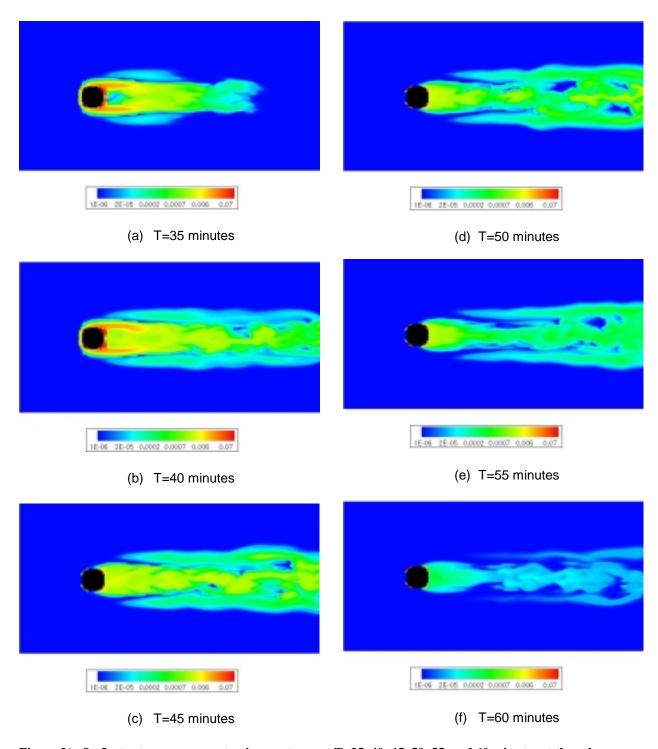


Figure 2(a-f). Instantaneous concentration contours at T=35, 40, 45, 50, 55, and 60 minutes at the release height, Z/H=0.778, using HIGRAD.

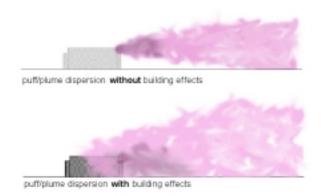


Figure 3. Building wake effects on dispersion.

dry deposition may be invoked as removal mechanisms. The Pasquill-Gifford dispersion scheme is used near source. Long travel time dispersion utilizes a scheme in which the growth of the puff is proportional to the square root of time. The implied modeling scale is from 10's of meters to 10's of kilometers.

## 4.2 Single, Elevated Source

A point source, 5 m in diameter, centered at 35m height, emitting 16g/s for 7.5 minutes was simulated for the "non-urban" or no building effects test case. The emission rate, emission time, and source height were based on an earlier CFD simulation. The wind speed was 3.5m/s and the stability class was D. A deposition velocity of 0.07cm/s was used so there would be some depositional loss of the pollutant. Downwind concentrations were all calculated at a height of 1.5m above ground. The receptor grid was spaced in units of 1/2 building length (60m) near the source and in greater increments of building length further downwind.

At 2.5 minutes, the maximum ground-level concentration occurred at 0.48 km, or four building lengths, downwind. At two building lengths (240 m) downwind from the source, the ground-level concentration is only 2% of the maximum. At 7.5 minutes, the time at which the source is shut off, high ground level concentration extends from 720 m to about 1.5 km. The relatively near-source concentration (240 m) is about 0.3% of the maximum.

These results are standard Gaussian plume results; with fixed wind direction the highest concentrations are on the plume centerline and with an elevated source in neutral conditions there is

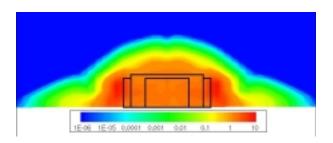


Figure 4. Y-Z cross-section of tracer dosage 1/4L downstream of the building simulated with HIGRAD.

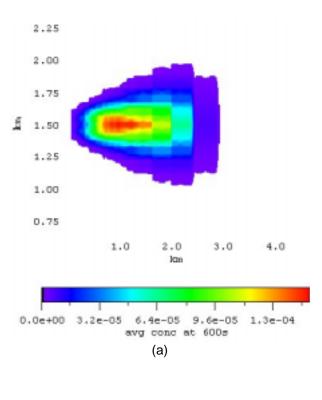
some gap distance before there is any ground level impact.

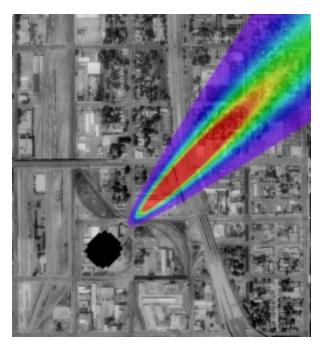
## 4.3 Three Source Simulation

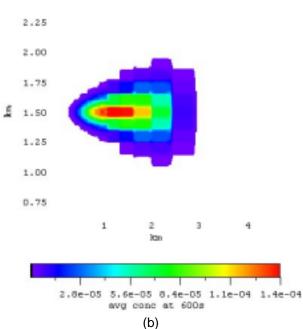
It is obvious from the CFD simulation that a one-source description cannot capture the building-induced behavior of the release. As shown in Figure 4, a Y-Z cross-section at 1/4L downwind of tracer dosage computed by HIGRAD, there are two "hot" spots on each side of the building. At this time we are testing the approach of modifying source characteristics to capture building effects rather than formally encoding building cavity and recirculation effects.

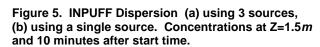
For the INPUFF model simulation, we have specified two intense sources at the building edges and a horizontally broad source at an elevation near the roofline. The two side sources were modeled as 25m high, centered at 25m elevation, and 10m wide. These were both given an intensity of 6g/s. The roofline source was modeled as 60m wide, 10m high, and centered at 45m elevation. This source had an intensity of 4g/s.

Figure 5 shows ground level concentrations of the three-source and one-source model simulations at 10 minutes. The boxiness of the plots results from the receptor spacing. The three-source model, as expected, results in ground level concentration close to the source (the first receptors were at 60*m*) and much higher ground level concentrations in the first kilometer. At fifteen minutes (after the source has been shut off) the three-source and one-source calculations begin to resemble each other, but the three-source calculation does show somewhat greater dispersion in both the x and y planes.









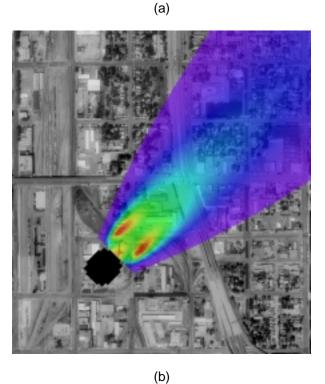


Figure 6. Gaussian plume model results for (a) a single source, and (b) 3 sources.

For a quick exercise, it was possible to capture some of the qualitative features of building effects with a three-source model. Whether with a different building and different source geometry it would be possible to do likewise with "expert" input separate from a CFD simulation remains to be determined.

### 4.4 The Gaussian Plume Model

The effects of the source characterization can also be seen in the plume spread of a Gaussian plume model. In Figures 6a and 6b, the impact of using the 3-source model is clearly seen. Figure 6a is the resultant dispersion from a single elevated source using rural plume spread parameters, where as Figure 6b is the dispersion using the HI-GRAD results to characterize 3 sources, including the building wake effects. Using the single source located at the building, the ground level concentration is zero for approximately 1L downstream, and the plume spread is much narrower. Using the 3 sources derived from the HIGRAD results, there are non-zero ground level concentrations near the building and the plume spread is much wider indicating a larger impacted area.

### 5.0 Conclusions

We have simulated the dispersion from HVAC vents for a large building, using 2 types of models. The first model, a large-eddy simulation code, was used to compute the near-source dispersion. The results were then used to characterize the source terms for a long-range Gaussian dispersion model, INPUFF, and in a Gaussian plume model. As shown, the non-Gaussian dispersion near the source, influenced by the presence of the building has an impact on the long-range dispersion. However, the largest difference from a single point source Gaussian dispersion model is nearest the building. As the pollutant advects farther from the source, the dispersion becomes more Gaussian.

Further research into the grid resolution effects and subgrid model was indicated. Additional simulations to quantify these effects are underway. In particular, we are doubling the resolution in all directions in order to determine what level of fidelity is required to capture the dominant effects of the dispersion.

Another consideration to be addressed in future simulations is the urban effects on dispersion around the building of interest. We are in the process of placing a city around our modeled

building so that the effects of adjacent building wakes on the flow may be assessed. It is anticipated that the adjacent building "wake effects" will substantially change the resultant dispersion from material released from the HVAC vents.

### 6.0 References

Brown, M.J., R.E. Lawson, D.S. DeCroix, R.L. Lee, 2000: Mean Flow and Turbulence Measurements Around a 2-D Array of Buildings in a Wind Tunnel. 11<sup>th</sup> AMS/AWMA J. Conf. Applic. of Air Poll. Meteor., Long Beach California, 9-14 January 2000.

Petersen, W.B. and L..G. Lavdas, 1986: INPUFF 2.0 - A Multiple Source Gaussian Puff Dispersion Algorithm. U.S. Environmental Protection Agency, EPA/600/8-86/024.

Smith, W.S., J.M. Reisner, D.S. DeCroix, M.J. Brown, R.L. Lee, S.T. Chan, D.E. Stevens, 2000: A CFD Model Intercomparison and Validation Using High resolution Wind Tunnel Data. 11<sup>th</sup> AMS/AWMA J. Conf. Applic. of Air Poll. Meteor., Long Beach California, 9-14 January 2000.

Smagorinsky, J., 1963: General circulation experiments with the primitive equations. 1: The basic experiment. *Mon. Wea. Rev.*, **91**, 99-164.

Smolarkiewicz, P. K., and W. H. Grabowski, 1990: The multidimensional positive definite advection transport algorithm: nonoscillatory option. J. Comp. Phys., **2**, 355-375.

Smolarkiewicz, P. K., and L. G. Margolin, 1993: On forward-in-time differencing for fluids: extension to a curvilinear framework. Mon. Wea. Rev., **121**, 1847-1859.

Smolarkiewicz, P. K., and L. G. Margolin, 1994: Variational solver for elliptic problems in atmospheric flows. Appl. Math. and Comp. Sci., **4**, 527-551.

Sorbjan, Z., 1996: Numerical Study of Penetrative and "Solid Lid" Nonpenetrative Convective Boundary Layers. J. Atmos. Sci., **53**, No. 1, 101-112.